Terascale Optimal PDE Simulations

TOPS @ Berkeley Lab

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What is TOPS

- TOPS = Terascale Optimal PDE Simulations.

- Funded by the Office of Advanced Scientific Computing Research (OASCR) of the Office of Science in the U.S. Department of Energy.
- Launched in July 2001 under the Scientific Discovery Through Advanced Computing (SciDAC) Program.
  - One of three applied math Integrated Software Infrastructure Centers (ISIC's).
  - One of 51 SciDAC projects in the Office of Science.

Goals of TOPS

TOPS
Terascale Optimal PDE Simulations

- Solver technology.
- Not just algorithms, but also vertically integrated software suites.
- Portable, scalable, extensible, tunable implementations.
- Starring ARPACK, Hypre, PETSc, SuperLU, and ScaLAPACK, among other existing packages.
- Motivated by representative applications, intended for many others.

Driving Force Behind TOPS

- Three driving SciDAC science applications in the original plan:
  - LBNL/SLAC-led "Advanced Computing for 21st Century Accelerator Science and Technology".
  - ORNL-led "Shedding New Light on Exploding Stars: Terascale Simulations of Neutrino-Driven SuperNovae and Their NucleoSynthesis".
  - PPPL-led "Extended Magnetohydrodynamic Modeling".
- Many more application partners now.
  - QCD, chemistry, …

Who are in TOPS

- Three DOE laboratories …
  - Argonne National Laboratory (Jorge Moré, Barry Smith)
  - Lawrence Berkeley National Laboratory (Esmond Ng)
  - Lawrence Livermore National Laboratory (Robert Falgout)
- Seven universities …
  - Carnegie Mellon University
  - Columbia University (David Keyes – lead PI)
  - New York University
  - Old Dominion University
  - University of California, Berkeley
  - University of Colorado, Boulder
  - University of Tennessee, Knoxville

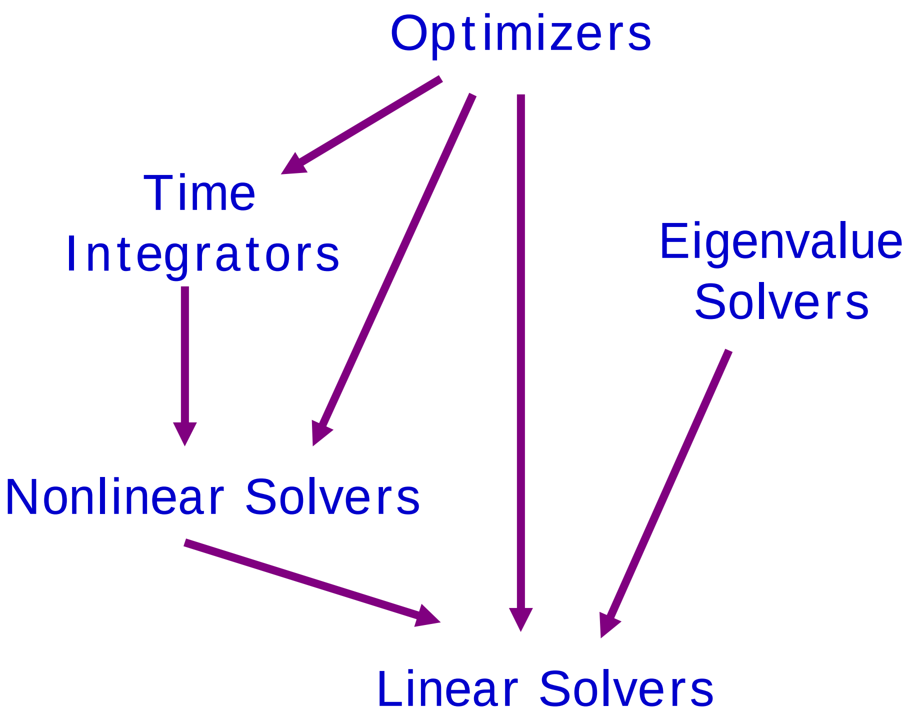
What Kind of Solvers

- Include:
  - Linear system solvers: $Ax = b$
  - Nonlinear implicit solvers: $F(x) = 0$
  - Adaptive time integrators for stiff systems: $f(x',x,t) = 0$
  - Optimizers: $\min_u \phi(x,u)$ s.t. $F(x,u) = 0$
  - Eigenvalue solvers: $Ax = \lambda Bx$

- Software integration.

- Performance optimization.

Scope of TOPS



→ Indicates dependence

TOPS @ Berkeley Lab

- Areas:
  - Linear Equations Solvers: $Ax = b$
    - Sparse direct methods
    - Preconditioning techniques for iterative methods
  - Eigenvalue Solvers: $Ax = \lambda Bx$

- Members:

Staff

Parry Husbands
Sherry Li
Osni Marques
Esmond Ng
Chao Yang

Postdocs

Laura Petrescu
Ali Pinar

Visiting Scientist

Weiguo Gao

Application Partners

- SLAC's Electromagnetic Systems Simulations in the Accelerator Science and Technology SciDAC Project.
  - Linear Algebra – large-scale sparse eigensolvers, sparse linear equations solvers (LBNL, Stanford, SLAC).
  - Load Balancing – improving performance and scalability (LBNL, Sandia, SLAC).
- Center for Extended Magnetohydrodynamic Modeling.
  - Linear Algebra – solution of large sparse ill-conditioned linear systems (LBNL, Univ. of Wisconsin).

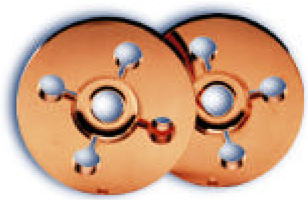
Designing Accelerator Structures

- Modeling of accelerator structures requires the solution of the Maxwell equations.

$$\nabla \times \mathrm{E} = -\frac{\partial \mathrm{B}}{\partial t}\,;\ \nabla \times H = -\frac{\partial \mathrm{D}}{\partial t}$$

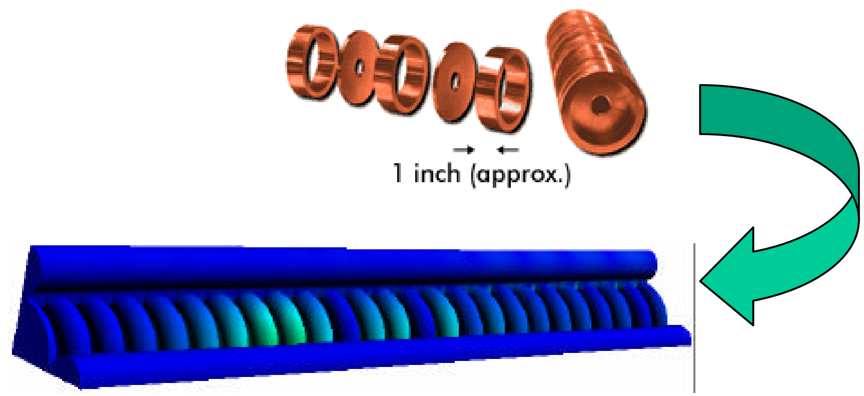
$$\nabla \cdot \mathrm{D} = 0\,;\ \nabla \cdot \mathrm{B} = 0$$

$$\mathrm{D} = e\mathrm{E}\,;\ \mathrm{B} = m\mathrm{H}$$



- Finite element discretization in frequency domain leads to a large sparse generalized eigenvalue problem.

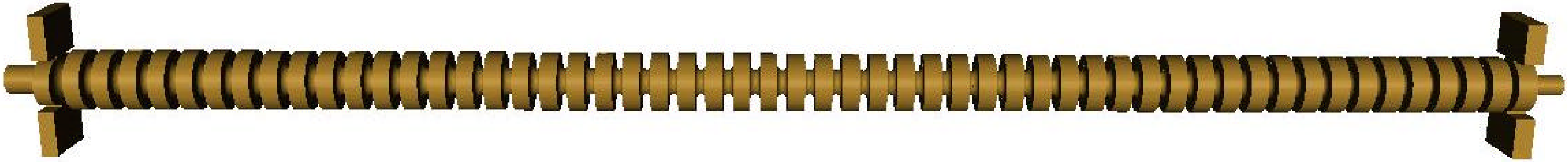
$$\mathrm{K}\,x = l\ \mathrm{M}\,x\ ,\ \ \mathrm{K} \geq 0;\ \mathrm{M} > 0$$



Designing Accelerator Structures

- Design of accelerator structures.
  - Modeling of a single accelerator cell suffices.
    - Relatively small eigenvalue problem.
  - There is an optimization problem here …
    - But need fast and reliable eigensolvers at every iteration.

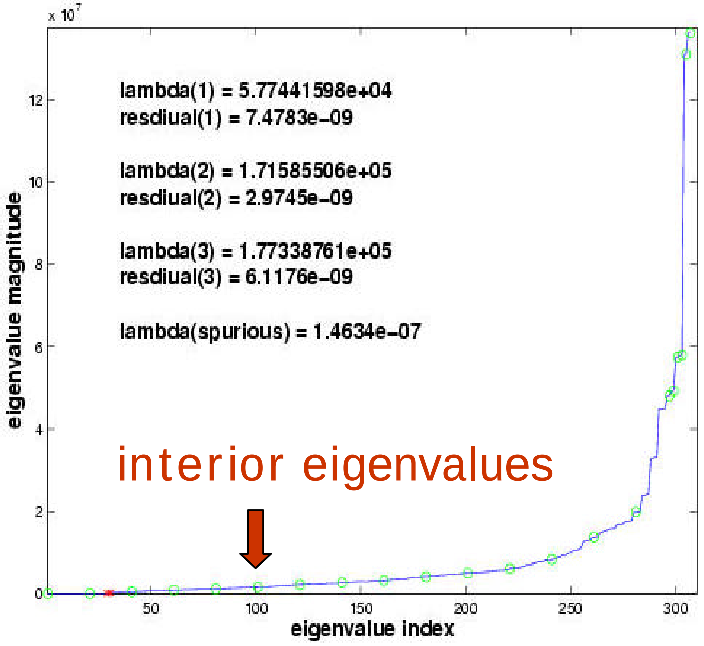
- Understanding the wake field requires the modeling of the full structure.
  - Need to compute a large number of frequency modes.



Challenges in Eigenvalue Calculations

- 3-D structures ⇒ large matrices.
  - Need very accurate interior eigenvalues that have relatively small magnitudes.
  - Eigenvalues are tightly clustered.
  - When losses in structures are considered, the problems will become complex symmetric.
- Omega3P has been able to compute eigen modes of large accelerator structures with large number of DOF's (without losses).

Spectral Distribution



Large-scale Eigenvalue Calculations

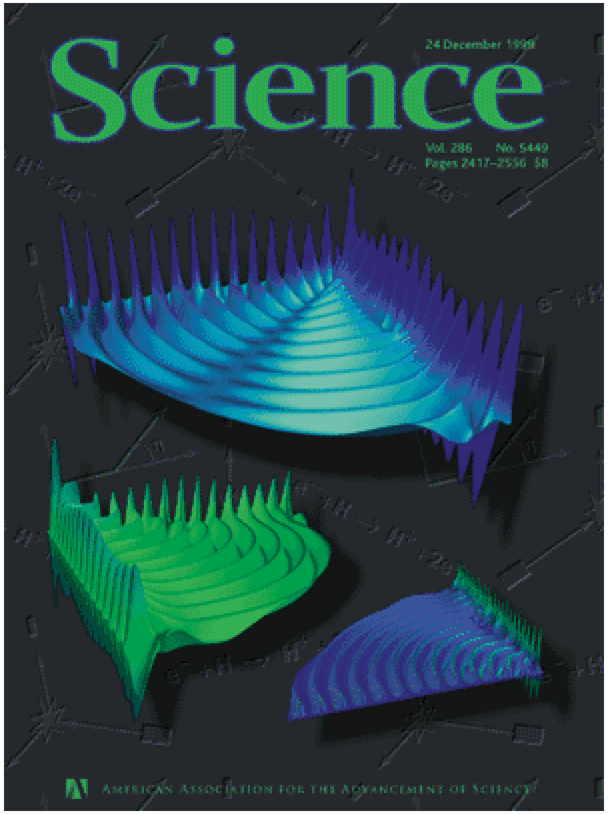
Terascale Optimal PDE Simulations

- Parallel shift-invert Lanczos algorithm.
  - Ideal for computing interior and clustered eigenvalues.

$$K x = \lambda M x \quad \rightarrow \quad M(K - \sigma M)^{-1} M x = \mu M x$$

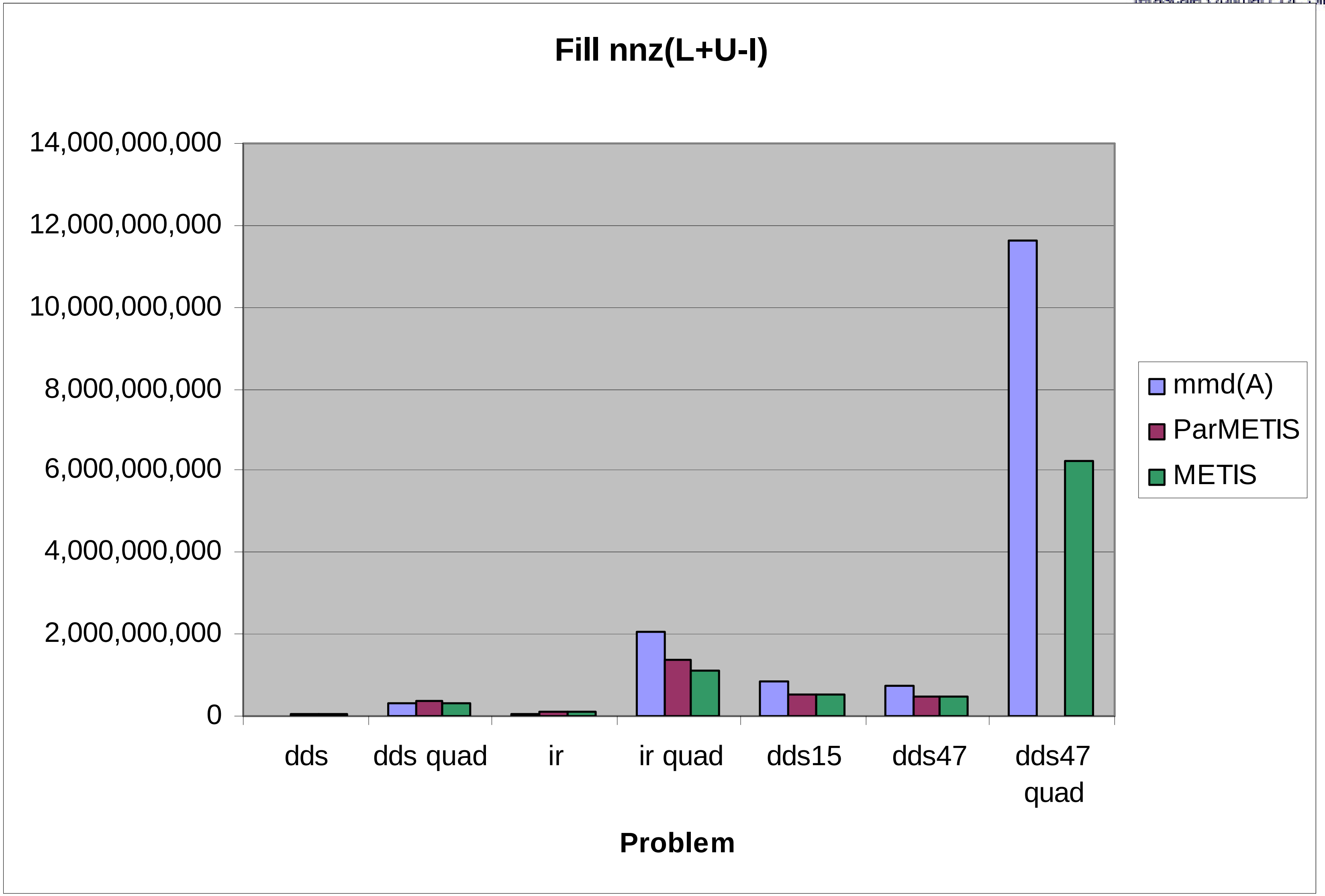
  - Need solution of sparse linear systems.
- SLAC: inexact solution + Newton-type correction.
- LBNL: exact shift-invert Lanczos.
  - Require complete factorizations of (sparse) matrices.
  - Exploit work on sparse direct solvers in TOPS.
  - Combine SuperLU_DIST with PARPACK to obtain a parallel implementation of a shift-invert Lanczos eigensolver.
  - Enable accurate calculation of eigenvalues, allow verification of other eigensolvers, and provide a baseline for comparisons.

High Performance Direct Linear Solver

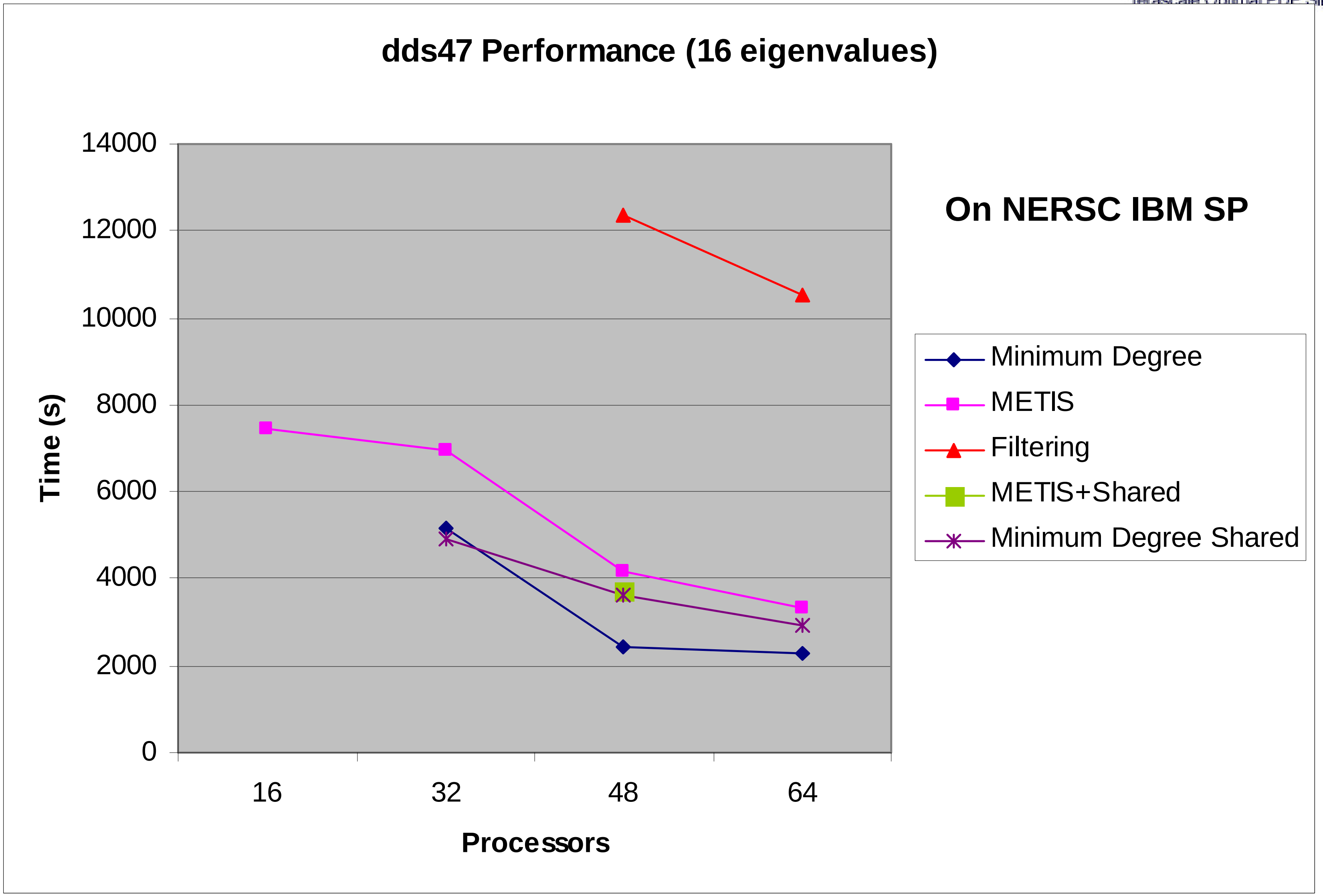


- SuperLU and SuperLU_Dist.
  - Direct solution of sparse linear system $Ax = b$.
  - Efficient, high-performance, portable implementations on modern computer architectures.
  - Support real and complex matrices, fill-reducing orderings, equilibration, numerical pivoting, condition estimation, iterative refinement, and error bounds.

Quick Tour of Results



Quick Tour of Results



Status of Eigenvalue Calculations

- Accomplishments:
  - TOPS/Exact Shift-invert Lanczos and Omega3P/Inexact Shift-invert Lanczos produce the same eigenvalues.
  - ESIL is faster than ISIL, but requires more memory.
    - NERSC IBM SP has >6 terabytes of real memory.
  - Exact shift-invert Lanczos has been integrated into Omega3P as a run-time option.

- The accelerator application helps motivate new developments & improvements in SuperLU.
  - Accommodate distributed input matrices.
  - Parallel symbolic factorization (in progress).
  - Improve triangular solution (in progress).

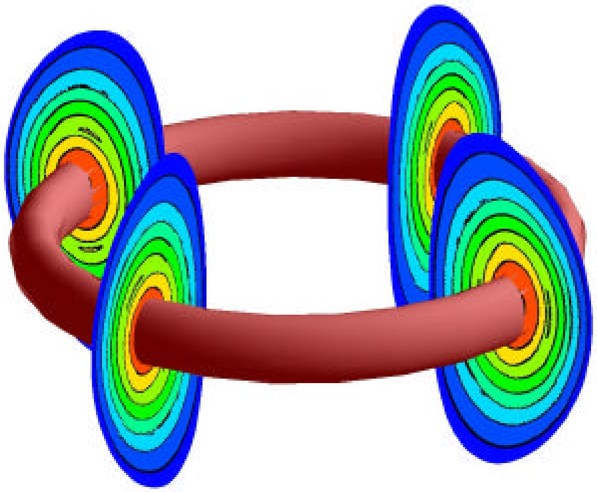
Highlights of Eigenvalue Calculations

- Largest eigensystem solved by LBNL team:
  - 7.5M DOFs, 304M nonzeros
  - 6,260M nonzeros in factors, requiring 2.5 hours to compute 10 eigenvalues close to a single shift using 24 processors (on 3 nodes) on NERSC IBM SP.

- Largest eigensystem solved by SLAC team:
  - > 90M DOFs with a sparse matrix factorization.

TOPS Meets Fusion

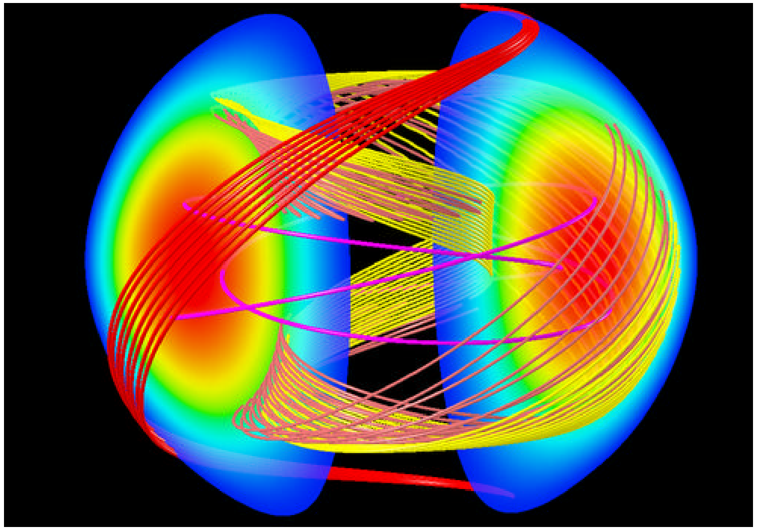
- NIMROD, developed at the Center for Extended Magnetohydrodynamic Modeling (CEMM), is a parallel simulation code for studying the nonlinear macroscopic electromagnetic dynamics in fusion plasmas.
  - Have difficulties in convergence when iterative methods are used in solving linear systems.



- Joint work between CEMM and TOPS has led to a performance improvement in NIMROD by a factor of 5-10 on NERSC IBM SP, "equivalent of 3-5 years progress in computing hardware" (Dalton Schnack of SAIC).

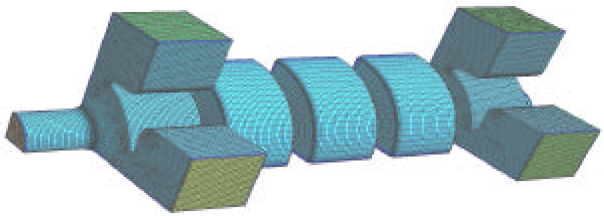
SuperLU Speeds Up Fusion Code

- Parallel SuperLU has been incorporated into NIMROD as an alternative linear solver.
  - In updating physical fields, SuperLU is used as a direct solver and is >100x and 64x faster on 1 and 9 processors, respectively.
  - A larger linear system in the time-advance has to be solved by the conjugate gradient method. SuperLU is used to factor a preconditioning matrix. This resulting in a 5-fold improvement in speed.

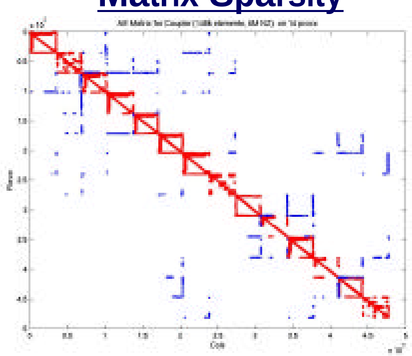


Load Balancing in EM Simulations

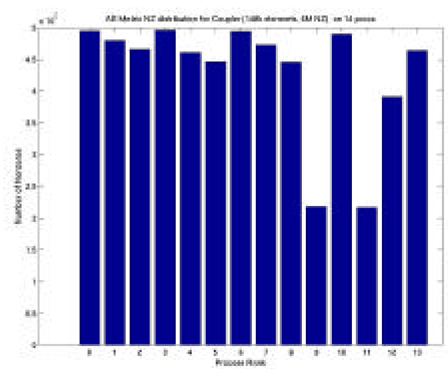
- Load balancing problem in Tau3P, a time-domain code for electromagnetic simulations.
  - Use of unstructured meshes and refinements lead to matrices for which nonzero entries are not evenly distributed.
  - Make work assignment and load balancing difficult in a parallel setting.
  - SLAC's Tau3P currently uses ParMETIS to partition the domain to minimize communication.



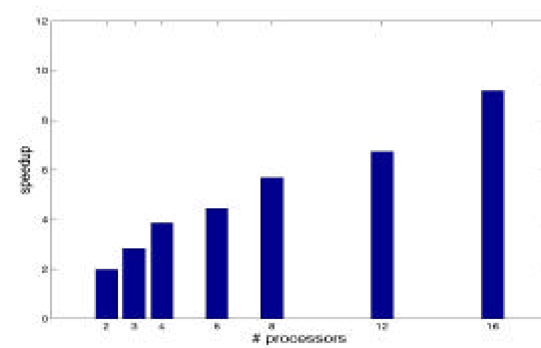
Matrix Sparsity



Matrix Distribution over 14 cpu's



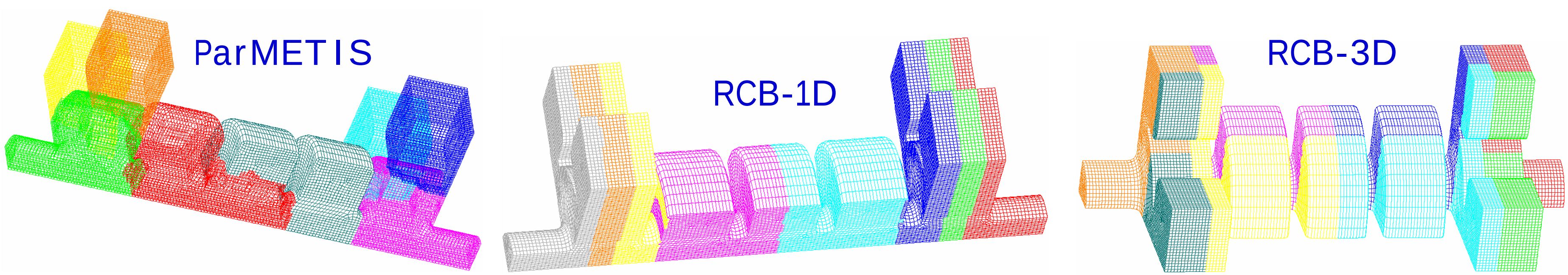
Parallel Speedup



Load Balancing in EM Simulations

- Collaboration between SLAC and TOPS (+ Sandia) has resulted in improved performance in Tau3P.
  - Sandia's Zoltan library is implemented to access better partitioning schemes for improved parallel performance over existing ParMETIS tool through reduced communication costs.

8 processor partitioning of a 5-cell RDDS with couplers on NERSC IBM SP			
	Tau3P Runtime	Max. Adj. Procs.	Max. Bound. Objects
ParMETIS	288.5 sec	3	585
RCB-1D	218.5 sec	2	3128
RCB-3D	345.6 sec	5	1965



Load Balancing in EM Simulations

ParMETIS

RCB-1D

Performance results on NERSC IBM SP for a 55-cell structure				
# of processors	ParMETIS run-time	ParMETIS max. adj. procs	RCB-1D run time	RCB-1D max. adj. procs
32	1455.0	4	1236.6	2
64	736.6	4	627.2	2
128	643.0	10	265.1	2
256	360.0	11	129.2	2
512	292.1	14	92.3	4

- Significant improvement obtained from using RCB-1D over ParMETIS on a 55-cell structure due to the linear nature of the geometry.

Summary and Future Plans

- TOPS/LBNL has contributed to great successes in some SciDAC applications.
- Future Plans:
  - Sparse direct solvers.
    - More improvements (e.g., symbolic factorization & triangular solutions) to make sparse direct methods more scalable.
    - Fill-reducing orderings and scheduling issues.
  - Eigenvalue calculations:
    - Other eigen solvers to handle extremely large problems (e.g., multilevel algorithms, Jacobi-Davidson).
  - Incomplete factorization algorithms for iterative methods.
  - Other applications.

- More information available at http://www.tops-scidac.org.